

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADO
NEWS	4	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	5	MAR 02	GBFULL: New full-text patent database on STN
NEWS	6	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	7	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	8	MAR 22	KOREAPAT now updated monthly; patent information enhanced
NEWS	9	MAR 22	Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS	10	MAR 22	PATDPASPC - New patent database available
NEWS	11	MAR 22	REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS	12	APR 04	EPFULL enhanced with additional patent information and new fields
NEWS	13	APR 04	EMBASE - Database reloaded and enhanced
NEWS	14	APR 18	New CAS Information Use Policies available online
NEWS	15	APR 25	Patent searching, including current-awareness alerts (SDIs), based on application date in CA/CAPLUS and USPATFULL/USPAT2 may be affected by a change in filing date for U.S. applications.
NEWS	16	APR 28	Improved searching of U.S. Patent Classifications for U.S. patent records in CA/CAPLUS
NEWS	17	MAY 23	GBFULL enhanced with patent drawing images
NEWS	18	MAY 23	REGISTRY has been enhanced with source information from CHEMCATS
NEWS	19	JUN 06	The Analysis Edition of STN Express with Discover! (Version 8.0 for Windows) now available
NEWS	20	JUN 13	RUSSIAPAT: New full-text patent database on STN
NEWS	21	JUN 13	FRFULL enhanced with patent drawing images
NEWS	22	JUN 27	MARPAT displays enhanced with expanded G-group definitions and text labels
NEWS	23	JUL 01	MEDICONF removed from STN
NEWS	24	JUL 07	STN Patent Forums to be held in July 2005
NEWS	25	JUL 13	SCISEARCH reloaded
NEWS	26	JUL 20	Powerful new interactive analysis and visualization software, STN AnaVist, now available
NEWS	27	AUG 11	Derwent World Patents Index(R) web-based training during August
NEWS	28	AUG 11	STN AnaVist workshops to be held in North America
NEWS EXPRESS			JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS INTER			General Internet Information
NEWS LOGIN			Welcome Banner and News Items
NEWS PHONE			Direct Dial and Telecommunication Network Access to STN
NEWS WWW			CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 10:08:42 ON 26 AUG 2005

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 10:08:50 ON 26 AUG 2005

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 AUG 2005 HIGHEST RN 861772-82-9

DICTIONARY FILE UPDATES: 24 AUG 2005 HIGHEST RN 861772-82-9

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TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

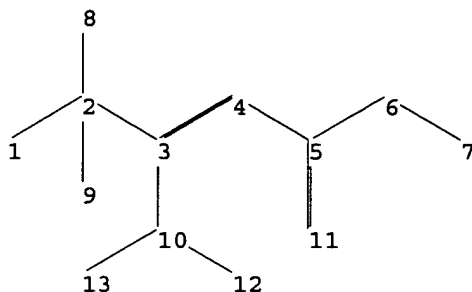
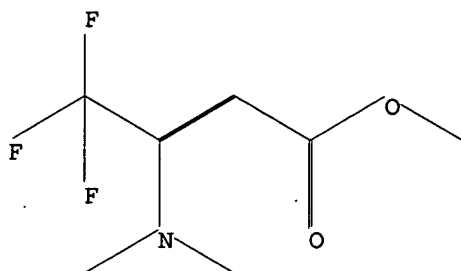
\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10511932\10511932 target cmpd.str



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

1-2 2-3 2-8 2-9 3-4 3-10 4-5 5-6 5-11 6-7 10-12 10-13

exact/norm bonds :

3-10 5-6 5-11 6-7 10-12 10-13

exact bonds :

1-2 2-3 2-8 2-9 3-4 4-5

Match level :

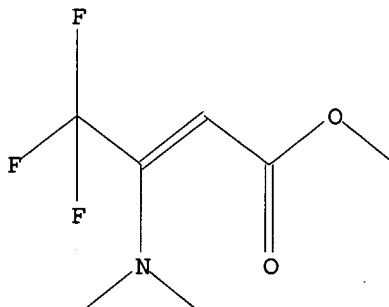
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS  
10:CLASS 11:CLASS 12:CLASS 13:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 11 sss sam

SAMPLE SEARCH INITIATED 10:09:25 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 36 TO ITERATE

100.0% PROCESSED 36 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 360 TO 1080

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> search l1 sss sam  
SAMPLE SEARCH INITIATED 10:14:43 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 36 TO ITERATE

100.0% PROCESSED 36 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 360 TO 1080  
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L1

=>

=> search l1 sss full  
FULL SEARCH INITIATED 10:15:04 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 593 TO ITERATE

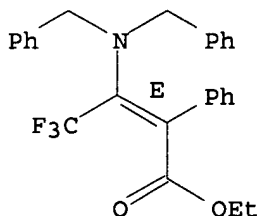
100.0% PROCESSED 593 ITERATIONS 8 ANSWERS  
SEARCH TIME: 00.00.01

L4 8 SEA SSS FUL L1

=> d scan

L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN Benzeneacetic acid,  $\alpha$ -[1-[bis(phenylmethyl)amino]-2,2,2-  
trifluoroethylidene]-, ethyl ester, ( $\alpha$ E)- (9CI)  
MF C26 H24 F3 N O2

Double bond geometry as shown.

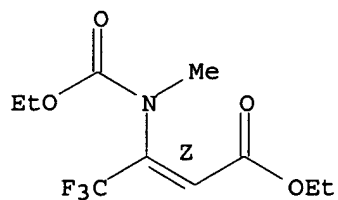


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):8

L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
IN 2-Butenoic acid, 3-[(ethoxycarbonyl)methylamino]-4,4,4-trifluoro-, ethyl  
ester, (2Z)- (9CI)  
MF C10 H14 F3 N O4

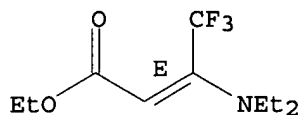
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 2-Butenoic acid, 3-(diethylamino)-4,4,4-trifluoro-, ethyl ester, (2E)-  
 (9CI)  
 MF C10 H16 F3 N O2

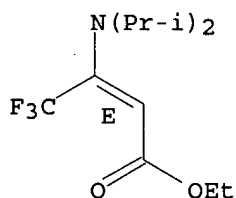
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 2-Butenoic acid, 3-[bis(1-methylethyl)amino]-4,4,4-trifluoro-, ethyl  
 ester, (2E)- (9CI)  
 MF C12 H20 F3 N O2

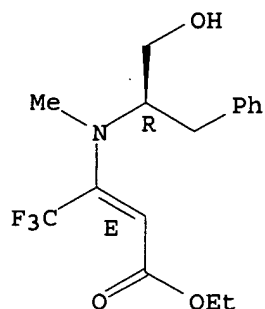
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 2-Butenoic acid, 4,4,4-trifluoro-3-[[[(1R)-1-(hydroxymethyl)-2-  
 phenylethyl]methylamino]-, ethyl ester, (2E)- (9CI)  
 MF C16 H20 F3 N O3

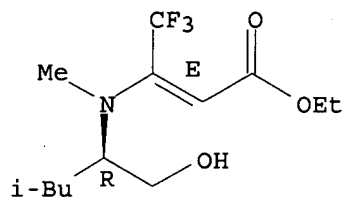
Absolute stereochemistry.  
 Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 2-Butenoic acid, 4,4,4-trifluoro-3-[[1R)-1-(hydroxymethyl)-3-methylbutyl]methylamino]-, ethyl ester, (2E)-(9CI)  
 MF C13 H22 F3 N O3

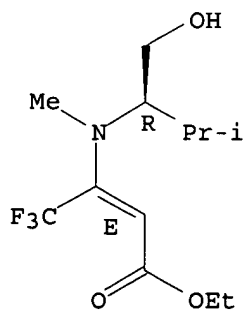
Absolute stereochemistry.  
 Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

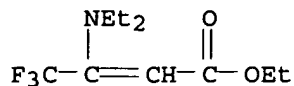
L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 2-Butenoic acid, 4,4,4-trifluoro-3-[[1R)-1-(hydroxymethyl)-2-methylpropyl]methylamino]-, ethyl ester, (2E)-(9CI)  
 MF C12 H20 F3 N O3

Absolute stereochemistry.  
 Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 8 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN  
 IN 2-Butenoic acid, 3-(diethylamino)-4,4,4-trifluoro-, ethyl ester (9CI)  
 MF C10 H16 F3 N O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus  
 COST IN U.S. DOLLARS  
 FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
166.06	166.27

FILE 'CAPLUS' ENTERED AT 10:16:14 ON 26 AUG 2005  
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FILE COVERS 1907 - 26 Aug 2005 VOL 143 ISS 10  
 FILE LAST UPDATED: 25 Aug 2005 (20050825/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l4

L5 5 L4

=> l4/prep

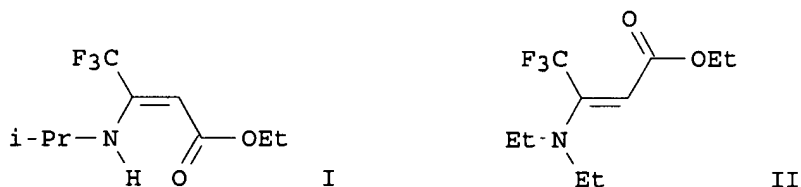
5 L4  
 3348673 PREP/RL  
 L6 4 L4/PREP  
 (L4 (L) PREP/RL)

=> d l6 1-4 ti fbib abs

L6 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN  
 TI A new synthesis of optically active 3-substituted (3S)-3,4-dihydro-5-(perfluoroalkyl)-2H-[1,4]oxazepin-7-ones  
 AN 2003:291077 CAPLUS  
 DN 139:117405  
 TI A new synthesis of optically active 3-substituted (3S)-3,4-dihydro-5-(perfluoroalkyl)-2H-[1,4]oxazepin-7-ones

AU Richard, Sebastien; Prie, Gildas; Guignard, Alain; Thibonnet, Jerome;  
 Parrain, J.-Luc; Duchene, Alain; Abarbri, Mohamed  
 CS Laboratoire de Physicochimie des Interfaces et des Milieux Reactionnels,  
 Faculte des Sciences de Tours, Tours, F-37200, Fr.  
 SO Helvetica Chimica Acta (2003), 86(3), 726-732  
 CODEN: HCACAV; ISSN: 0018-019X  
 PB Verlag Helvetica Chimica Acta  
 DT Journal  
 LA English  
 OS CASREACT 139:117405  
 AB Optically active (perfluoroalkyl)-oxazepin-7-ones were synthesized in two  
 steps starting from Et perfluorobut-2-ynoate by direct addition of optically  
 active amino alcs. via intermol. Michael addition and lactone formation.  
 RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

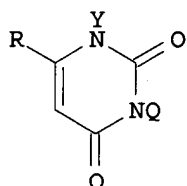
L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN  
 TI Easy synthesis of (E)- or (Z)-perfluorinated  $\beta$ -enaminoesters  
 AN 2002:732461 CAPLUS  
 DN 138:187392  
 TI Easy synthesis of (E)- or (Z)-perfluorinated  $\beta$ -enaminoesters  
 AU Prie, Gildas; Richard, Sebastien; Parrain, Jean-Luc; Duchene, Alain;  
 Abarbri, Mohamed  
 CS Faculte des Sciences de Tours, Laboratoire de Physicochimie des Interfaces  
 et des Milieux Reactionnels, Tours, 37200, Fr.  
 SO Journal of Fluorine Chemistry (2002), 117(1), 35-41  
 CODEN: JFLCAR; ISSN: 0022-1139  
 PB Elsevier Science B.V.  
 DT Journal  
 LA English  
 OS CASREACT 138:187392  
 GI



AB (E)- or (Z)-perfluorinated  $\beta$ -enaminoesters, e.g. I and II, were  
 prepared by direct addition of primary or secondary amines to Et  
 perfluoroalkynoates without any catalyst.  
 RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN  
 TI Preparation of 6-(perfluoroalkyl)uracils from 3-(alkoxycarbonylamino)-3-  
 perfluoroalkylacrylates and amines.  
 AN 2000:592705 CAPLUS  
 DN 133:177187  
 TI Preparation of 6-(perfluoroalkyl)uracils from 3-(alkoxycarbonylamino)-3-  
 perfluoroalkylacrylates and amines.  
 IN Kameswaran, Venkataraman  
 PA American Cyanamid Company, USA  
 SO PCT Int. Appl., 91 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1  
 PATENT NO.                      KIND      DATE                      APPLICATION NO.                      DATE

PI	WO 2000049003	A1	20000824	WO 2000-US3795	20000214
	W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	CA 2362996	AA	20000824	US 1999-250725	A 19990216
				CA 2000-2362996	20000214
				US 1999-250725	A 19990216
				WO 2000-US3795	W 20000214
	EP 1150962	A1	20011107	EP 2000-911810	20000214
	EP 1150962	B1	20040428		
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
				US 1999-250725	A 19990216
				WO 2000-US3795	W 20000214
	BR 2000008306	A	20020122	BR 2000-8306	20000214
				US 1999-250725	A 19990216
				WO 2000-US3795	W 20000214
	JP 2002537290	T2	20021105	JP 2000-599743	20000214
				US 1999-250725	A 19990216
				WO 2000-US3795	W 20000214
	AT 265440	E	20040515	AT 2000-911810	20000214
				US 1999-250725	A 19990216
				WO 2000-US3795	W 20000214
OS	CASREACT 133:177187; MARPAT 133:177187				
GI					



I

AB Title compds. [I; R = CnF2n+1; n = 1-6; Y = H, alkyl; Q = alkyl, (substituted) Ph, PhCH2, heteroaryl, methyleneheteroaryl], were prepared by reaction of CnF2n+1C(:CHCO2Z1)N(Y)CO2Z [Z, Z1 = alkyl, (substituted) PhCH2; n, Y as above] with QNH2 in the presence of base followed by optional alkylation. Thus, Et [(ethoxycarbonyl)amino]-4,4,4-trifluorocrotonate (preparation given), Me2CHNH2, and DBU were refluxed in xylene to give 61% 3-isopropyl-6-trifluoromethyl-2,4-(1H,3H)-pyrimidinedione.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

TI Concise stereoselective synthesis of 1-perfluoroalkyl enamines via the addition of N-lithiated amines to enol ethers and their subsequent metalation to form new functionalized enamines

AN 1998:317130 CAPLUS

DN 129:95082

TI Concise stereoselective synthesis of 1-perfluoroalkyl enamines via the addition of N-lithiated amines to enol ethers and their subsequent metalation to form new functionalized enamines

AU Begue, Jean-Pierre; Bonnet-Delpon, Daniele; Bouvet, Denis; Rock, Michael

H.  
 CS Centre d'Etudes Pharmaceutiques, BioCIS-CNRS, Chatenay-Malabry, F-92296, Fr.  
 SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1998), (11), 1797-1800  
 CODEN: JCPRB4; ISSN: 0300-922X  
 PB Royal Society of Chemistry  
 DT Journal  
 LA English  
 OS CASREACT 129:95082  
 AB Addition of lithium amides, e.g., (PhCH<sub>2</sub>)<sub>2</sub>NLi, derived from a range of cyclic, sterically demanding, and chiral amines, to trifluoromethyl (Z)-enol ethers, e.g., (Z)-F<sub>3</sub>CC(OEt):CHPh and (Z)-F<sub>3</sub>CC(OEt):CHC<sub>6</sub>H<sub>4</sub>OMe-4, gave stereoselectively the corresponding (Z)- enamines, e.g. (Z)-(PhCH<sub>2</sub>)<sub>2</sub>NC(CF<sub>3</sub>):CHPh and (Z)-(PhCH<sub>2</sub>)<sub>2</sub>NC(CF<sub>3</sub>):CHC<sub>6</sub>H<sub>4</sub>OMe-4, in good yields. The reaction was extended to perfluoroalkyl and chlorofluoroalkyl enol ethers, e.g., EtOC(CClF<sub>2</sub>):CHPh. The enamines react with Me<sub>3</sub>CLi to give vinylic anions and, after quenching with aldehydes and Et chloroformate, provide new functionalized enamines, e.g., (PhCH<sub>2</sub>)<sub>2</sub>NC(CF<sub>3</sub>):C(Ph)CH(OH)Et.  
 RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> trifluoroacetate  
       8419 TRIFLUOROACETATE  
       818 TRIFLUOROACETATES  
 L7      8790 TRIFLUOROACETATE  
           (TRIFLUOROACETATE OR TRIFLUOROACETATES)

=> 16 and 17  
 L8      0 L6 AND L7

=> FIL CASREACT

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	17.98	184.25
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.92	-2.92

FILE 'CASREACT' ENTERED AT 10:21:01 ON 26 AUG 2005  
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FILE CONTENT:1840 - 21 Aug 2005 VOL 143 ISS 8

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*****
*
*   CASREACT now has more than 9.2 million reactions
*
*****

```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> SET NOTICE DISPLAY 1

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=> D ACC 138:187392 ALL

THE ESTIMATED COST FOR THIS REQUEST IS 6.62 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:n  
REQUEST CANCELED

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.43	184.68
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-2.92

SESSION WILL BE HELD FOR 60 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 10:21:26 ON 26 AUG 2005

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
SESSION RESUMED IN FILE 'CASREACT' AT 10:55:30 ON 26 AUG 2005  
FILE 'CASREACT' ENTERED AT 10:55:30 ON 26 AUG 2005  
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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.43	184.68
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-2.92

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.43	184.68
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-2.92

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 10:55:43 ON 26 AUG 2005

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
SESSION RESUMED IN FILE 'CASREACT' AT 11:22:56 ON 26 AUG 2005  
FILE 'CASREACT' ENTERED AT 11:22:56 ON 26 AUG 2005  
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.43	184.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.92

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.43	184.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.92

FILE 'REGISTRY' ENTERED AT 11:23:02 ON 26 AUG 2005  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 AUG 2005 HIGHEST RN 861772-82-9  
DICTIONARY FILE UPDATES: 24 AUG 2005 HIGHEST RN 861772-82-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more

information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> e ethyl-4,4,4-trifluoroacetoacetate/cn

E1	1	ETHYL-3-PROPOXYBENZIMIDATE/CN
E2	1	ETHYL-4,12-TRIDECADIENOATE/CN
E3	0 -->	ETHYL-4,4,4-TRIFLUOROACETOACETATE/CN
E4	1	ETHYL-4,6-DI-O-ACETYL-A-Ψ-D-GLUCAL/CN
E5	1	ETHYL-4,6-DI-O-ACETYL-2,3-DIDEOXY-A-D-ERYTHROHEX-2-ENO PYRANOSIDE/CN
E6	1	ETHYL-4-(9-(1-ETHYL-4(1H)-QUINOLYLIDENE)-5-HYDROXY-1,3,5,7-N ONATETRAENYL)-1-QUINOLINIUM PERCHLORATE, ACETATE/CN
E7	1	ETHYL-4-ACETYL-3,5-DIMETHYLPYRROLE-2-CARBOXYLATE/CN
E8	1	ETHYL-4-BROMO-2,5-DICHLOROPHENYL PHOSPHOROTHIONATE/CN
E9	1	ETHYL-4-GUANIDINO BENZOATE/CN
E10	1	ETHYL-4-METHYLDIBENZOTHIOPHENE/CN
E11	1	ETHYL-4H-1,2,4-TRIAZOLE-4-CARBAMATE/CN
E12	1	ETHYL-6-AMINO-3,4-DIISOBUTOXYBENZOATE/CN

=> e ethyl-4,4,4-trifluoroacetoacetate/cn

E1	1	ETHYL-3-PROPOXYBENZIMIDATE/CN
E2	1	ETHYL-4,12-TRIDECADIENOATE/CN
E3	0 -->	ETHYL-4,4,4-TRIFLUOROACETOACETATE/CN
E4	1	ETHYL-4,6-DI-O-ACETYL-A-Ψ-D-GLUCAL/CN
E5	1	ETHYL-4,6-DI-O-ACETYL-2,3-DIDEOXY-A-D-ERYTHROHEX-2-ENO PYRANOSIDE/CN
E6	1	ETHYL-4-(9-(1-ETHYL-4(1H)-QUINOLYLIDENE)-5-HYDROXY-1,3,5,7-N ONATETRAENYL)-1-QUINOLINIUM PERCHLORATE, ACETATE/CN
E7	1	ETHYL-4-ACETYL-3,5-DIMETHYLPYRROLE-2-CARBOXYLATE/CN
E8	1	ETHYL-4-BROMO-2,5-DICHLOROPHENYL PHOSPHOROTHIONATE/CN
E9	1	ETHYL-4-GUANIDINO BENZOATE/CN
E10	1	ETHYL-4-METHYLDIBENZOTHIOPHENE/CN
E11	1	ETHYL-4H-1,2,4-TRIAZOLE-4-CARBAMATE/CN
E12	1	ETHYL-6-AMINO-3,4-DIISOBUTOXYBENZOATE/CN

=> e ethyl 4,4,4-trifluoroacetoacetate/cn

E1	1	ETHYL 4,4,4-TRIFLUORO-3-OXOBUTANOATE/CN
E2	1	ETHYL 4,4,4-TRIFLUORO-3-OXOBUTYRATE/CN
E3	1 -->	ETHYL 4,4,4-TRIFLUOROACETOACETATE/CN
E4	1	ETHYL 4,4,4-TRIFLUOROACETYLACETONATE/CN
E5	1	ETHYL 4,4,4-TRIFLUOROBUTANOATE/CN
E6	1	ETHYL 4,4,4-TRIFLUOROBUTYRATE/CN
E7	1	ETHYL 4,4,4-TRIFLUOROCROTONATE/CN
E8	1	ETHYL 4,4,4-TRINITROBUTYRATE/CN
E9	1	ETHYL 4,4,5,5,5-PENTAFLUORO-3-METHOXY-2-PENTENOATE/CN
E10	1	ETHYL 4,4,5,5,5-PENTAFLUORO-3-OXOPENTANOATE/CN
E11	1	ETHYL 4,4,5,5,5-PENTAFLUORO-3-OXOVALERATE/CN
E12	1	ETHYL 4,4,5,5-TETRAFLUORO-3-OXOPENTANOATE/CN

=> e3

L9 1 "ETHYL 4,4,4-TRIFLUOROACETOACETATE"/CN

=> d 19

L9 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN

RN 372-31-6 REGISTRY

ED Entered STN: 16 Nov 1984

CN Butanoic acid, 4,4,4-trifluoro-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Acetoacetic acid, 4,4,4-trifluoro-, ethyl ester (6CI, 8CI)

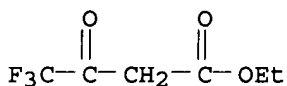
OTHER NAMES:

CN 1-Ethoxy-4,4,4-trifluorobutane-1,3-dione

CN 4,4,4-Trifluoro-3-oxobutanoic acid ethyl ester

CN 4,4,4-Trifluoroacetoacetic acid ethyl ester

CN Ethyl (trifluoroacetyl)acetate  
 CN Ethyl  $\gamma,\gamma,\gamma$ -trifluoroacetoacetate  
 CN Ethyl  $\omega,\omega,\omega$ -trifluoroacetoacetate  
 CN Ethyl 3-oxo-4,4,4-trifluorobutanoate  
 CN Ethyl 4,4,4-trifluoro-3-oxobutanoate  
 CN Ethyl 4,4,4-trifluoro-3-oxobutyrate  
 CN **Ethyl 4,4,4-trifluoroacetoacetate**  
 CN Ethyl 4,4,4-trifluoroacetylacetonate  
 CN Ethyl trifluoroacetoacetate  
 CN NSC 42739  
 CN NSC 49750  
 FS 3D CONCORD  
 MF C6 H7 F3 O3  
 CI COM  
 LC STN Files: AGRICOLA, BEILSTEIN\*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS,  
 CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHM, GMELIN\*,  
 HODOC\*, IFICDB, IFIPAT, IFIUDB, PS, SPECINFO, SYNTHLINE, TOXCENTER,  
 USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)  
 Other Sources: EINECS\*\*, NDSL\*\*, TSCA\*\*  
 (\*\*Enter CHEMLIST File for up-to-date regulatory information)



**\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\***

616 REFERENCES IN FILE CA (1907 TO DATE)  
 9 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 616 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 25 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.73	192.41
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.92

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FILE COVERS 1907 - 26 Aug 2005 VOL 143 ISS 10  
 FILE LAST UPDATED: 25 Aug 2005 (20050825/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l9/prep

616 L9  
3348673 PREP/RL  
L10 26 L9/PREP  
(L9 (L) PREP/RL)

=> alkoxide

18843 ALKOXIDE  
14664 ALKOXIDES  
L11 26898 ALKOXIDE  
(ALKOXIDE OR ALKOXIDES)

=> l10 and l11

L12 0 L10 AND L11

=> ?oxide

L13 2564126 ?OXIDE

=> l10 and l12

L14 0 L10 AND L12

=> claiasen

0 CLAIASEN  
L15 0 CLAIASEN

=> claisen

6500 CLAISEN  
3 CLAISENS  
L16 6502 CLAISEN  
(CLAISEN OR CLAISENS)

=> l10 and l16

L17 3 L10 AND L16

=> d l17 1-3 ti fbib abs

L17 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

TI Manufacture of alkyl trifluoroacetoacetate

AN 1988:612818 CAPLUS

DN 109:212818

TI Manufacture of alkyl trifluoroacetoacetate

IN Mysinsky, Edward

PA Monsanto Co., Japan

SO Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 63156753	A2	19880629	JP 1986-298587	19861215
	JP 05029344	B4	19930430		
				JP 1986-298587	19861215

AB The title compds. are prepared by reacting C1-5 alkyl 3-alkoxy-3-hydroxy-4,4,4-trifluorobutanoate (I) with acetyl halide or Ac2O under pressure at a temperature  $\geq 10^\circ$  but lower than the reflux temperature of the reaction mixture Adding 79.0 parts Et trifluoroacetate to 61.8 parts cyclohexane (II) and 22.3 parts NaOH (as 60% mineral oil dispersion), heating with 53.9 parts EtOAc for 2 h at 45-60°, diluting with 55.7 parts II, neutralizing with HCl, refluxing the slurry with 41.5 parts CH3COCl,

filtering, washing and distilling provided 75% Et trifluoroacetoacetate.

L17 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

TI Preparation of alkyl trifluoroacetoacetate

AN 1987:439216 CAPLUS

DN 107:39216

TI Preparation of alkyl trifluoroacetoacetate

IN Micinski, Edward

PA Monsanto Co. , USA

SO U.S., 6 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4647689	A	19870303	US 1982-403754	19820730
	CA 1284153	A1	19910514	CA 1986-524197	19861201
				US 1982-403754	19820730
	AU 591536	B2	19891207	AU 1986-66060	19861203
	AU 8666060	A1	19880609		
				US 1982-403754	19820730
	EP 270724	A1	19880615	EP 1986-870187	19861212
	EP 270724	B1	19901128		
	R: AT, BE, CH, DE, ES, FR, GB, IT, LI, LU, NL, SE				
				US 1982-403754	19820730
	AT 58719	E	19901215	AT 1986-870187	19861212
				EP 1986-870187	A 19861212

OS CASREACT 107:39216

AB The title C1-5 alkyl trifluoroacetoacetates (I) are prepared by acetylation of C1-5 alkyl 3-alkoxy-3-hydroxy-4,4,4-trifluorobutanoate obtained from **Claisen** condensation of alkyl trifluoroacetate and alkyl acetate in the presence of a strong base. F3CCO2Et was condensed with EtOAc in the presence of NaH to give a mixture containing EtOH and F3COCH2CO2Et.Na, which

was

neutralized with HCl to give F3CC(OH)(OEt)CH2CO2Et, treatment of which with AcCl gave 75% F3CCOCH2COEt.

L17 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

TI Synthesis and spectral study of 4-(perfluoroalkyl)coumarins

AN 1982:544728 CAPLUS

DN 97:144728

TI Synthesis and spectral study of 4-(perfluoroalkyl)coumarins

AU Bayer, V.; Pastor, R.; Cambon, A.

CS Fac. Sci., Unites Enseign. Rech., Nice, 06034, Fr.

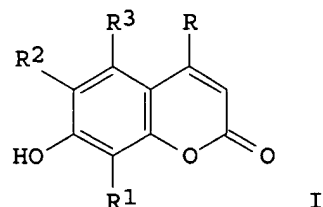
SO Journal of Fluorine Chemistry (1982), 20(2), 187-202

CODEN: JFLCAR; ISSN: 0022-1139

DT Journal

LA French

GI



AB Coumarins I [R = (CF<sub>2</sub>)<sub>n</sub>CF<sub>3</sub> (n = 0, 2, 4, 6); R<sub>1</sub> = H, OH, Me; R<sub>2</sub>, R<sub>3</sub> = H, OH] were obtained by treating RCOCH<sub>2</sub>CO<sub>2</sub>Et with phenols. RCOCH<sub>2</sub>CO<sub>2</sub>Et were prepared by Claisen condensation of RCO<sub>2</sub>Et with EtOAc. The <sup>1</sup>H and <sup>19</sup>F-NMR spectra of I are discussed. A new long distance H-F coupling constant [5J] was observed and interpreted as a coupling through space.

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	21.45	213.86
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.19	-5.11

SESSION WILL BE HELD FOR 60 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 11:30:10 ON 26 AUG 2005

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
SESSION RESUMED IN FILE 'CAPLUS' AT 12:22:09 ON 26 AUG 2005  
FILE 'CAPLUS' ENTERED AT 12:22:09 ON 26 AUG 2005  
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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	21.45	213.86
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.19	-5.11

=> d his

(FILE 'HOME' ENTERED AT 10:08:42 ON 26 AUG 2005)

FILE 'REGISTRY' ENTERED AT 10:08:50 ON 26 AUG 2005

L1 STRUCTURE UPLOADED  
L2 0 SEARCH L1 SSS SAM  
L3 0 SEARCH L1 SSS SAM  
L4 8 SEARCH L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:16:14 ON 26 AUG 2005

L5 5 L4  
L6 4 L4/PREP  
L7 8790 TRIFLUOROACETATE  
L8 0 L6 AND L7

FILE 'CASREACT' ENTERED AT 10:21:01 ON 26 AUG 2005

SET NOTICE DISPLAY 1  
SET NOTICE LOGIN DISPLAY

FILE 'REGISTRY' ENTERED AT 11:23:02 ON 26 AUG 2005

E ETHYL-4,4,4-TRIFLUOROACETOACETATE/CN  
E ETHYL-4,4,4-TRIFLUOROACETOACETATE/CN

E ETHYL 4,4,4-TRIFLUOROACETOACETATE/CN

L9

1 E3

FILE 'CAPLUS' ENTERED AT 11:25:03 ON 26 AUG 2005

L10 26 L9/PREP  
L11 26898 ALKOXIDE  
L12 0 L10 AND L11  
L13 2564126 ?OXIDE  
L14 0 L10 AND L12  
L15 0 CLAIASEN  
L16 6502 CLAISEN  
L17 3 L10 AND L16

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

21.90

214.31

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-2.19

-5.11

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 12:22:27 ON 26 AUG 2005